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STABILITY AND UNIQUENESS IN NONLINEAR CONTINUUM  
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MATHEMATICS M E GURTIN 08 JAN 88 ARO-21802 11-MA

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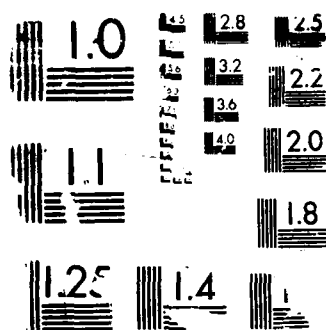
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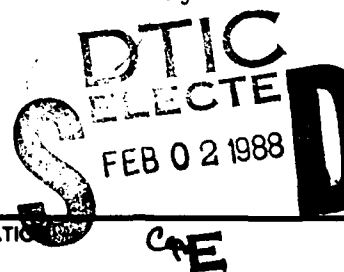




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The main thrust of this project was to develop a thermodynamically admissible theory of phase transitions, hopefully appropriate for the study of crystal growth. Secondary projects included the development of models for thermoviscoelasticity and thermoviscoplasticity.



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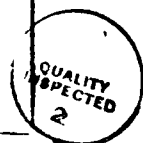
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**Stability and Uniqueness in Nonlinear  
Continuum Mechanics**

**Final Report**

**Morton E. Gurtin**

**January 8, 1988**

**U.S. Army Research Office**

**ARO Grant DAAG29-85-K-0004**

**Department of Mathematics  
Carnegie Mellon University  
Pittsburgh, PA 15213**

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**Problems Studied**

The main thrust of this project was to develop a thermodynamically admissible theory of phase transitions, hopefully appropriate for the study of crystal growth. Secondary projects included the development of models for thermoviscoelasticity and thermoviscoplasticity.

## Summary of Results

### Solidification

The classical theory of Stefan, for the melting of a solid or the freezing of a liquid, is far too simplistic to account for the myriad of phenomena<sup>1</sup> which occur during solidification (an example being dendritic growth, in which simple shapes evolve to complicated tree-like structures). Motivated by work of Mullins and Sekerka [R1,R2], a continuum theory of melting and solidification - of sufficient generality to model phenomena of this type - was developed [Q4,Q12] (see also the review [Q8]). The theory starts from general (nonequilibrium) thermodynamical laws which are appropriate to a continuum and which include contributions of energy and entropy for the interface between phases. Among the results is an interface condition (generalizing the classical Gibbs-Thompson equation) which relates the temperature at the interface to: the jumps in energy and entropy across the interface, the interfacial values of energy and entropy, the interfacial curvature. This result is independent of particular constitutive equations and shows that whenever the interface is endowed with energy and entropy, the temperature must necessarily be a function of curvature.

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<sup>1</sup>Chalmers [R3], Delves [R4], and Doherty [R5] discuss these phenomena.

Constitutive equations for the interface, of sufficient generality to describe crystal growth involving an anisotropic material structure, are introduced; and corresponding restrictions, necessary and sufficient for compatibility with thermodynamics, are found [Q12].

Using these restrictions appropriate free-boundary conditions for the interface are developed, and various physically-realistic free-boundary problems are described. These generalize the classical Stefan problem, the Mullins-Sekerka problem [R1,R2] resulting when interfacial energy and entropy are small. It is shown that (within the Mullins-Sekerka theory) the volume  $V(t)$  and surface area  $A(t)$ , of a body of arbitrary shape solidifying in a melt of uniform far-field temperature, satisfy:

$$\frac{d}{dt} [A(t) + cV(t)] \leq 0,$$

with  $c$  a constant which is negative when the far-field is supercooled, but otherwise positive.

We also study the corresponding equilibrium theory and show [Q4] that in certain situations there are no global energy minimizers, but there are minimizing sequences, and these seem consistent with instabilities such as the formation of complicated arrays of thin spikes, behavior which may be indicative of dendritic growth.

We believe the theory developed in [Q4] will have many



applications. For example, morphological instabilities such as dendritic growth, along with the microsegregation of solutes or impurities that usually accompany them, determine the microstructure and defect structure of the growing phase. Since this structure has a strong influence on material properties, such instabilities play an important role in materials science. Examples are most prevalent in the casting of metal alloys and in the growth of semiconductor crystals from the melt, but are also associated with laser, magnetic, piezoelectric and other crystals. Moreover, this is not the only field of science in which these ideas may be important: for example, in the study of precipitated snow the conversion of dendrites of snow into sets of isolated arms, due to a rise in temperature, is believed to be a cause of some snow avalanches (cf. the discussion by Doherty [R5]).

### Theories of phase equilibria

The classical theory of phase transitions in fluids consists in minimizing the total energy over all density fields with given total mass. The chief difficulty with this approach is the existence of an infinity of solutions involving an arbitrary number of transitions between constant states.

To remedy this difficulty we have developed [Q1,Q9] a theory in which transitions between phases are accompanied by

an increase in energy proportional to interfacial area (i.e. to the area of the surface separating the two phases). The theory also includes contact energy between each of the phases and the confining vessel. Within this framework a two-phase fluid of total mass  $m$  confined to a container  $\Omega$  will have stable density distributions  $u = u(x)$  characterized by the variational problem

$$\begin{aligned} \text{VP:} \quad & \text{minimize} \quad \sigma A(u) + \sum \sigma_i A_i(u) + \sum \int_{\Omega} W_i(u) \\ & \text{subject to} \quad \int_{\Omega} u = m. \end{aligned}$$

Here  $W_i(u)$  represents the free energy of phase  $i$  ( $i=1,2$ ).  $A(u)$  is the area of the interface between phases,  $A_i(u)$  is the contact area between phase  $i$  and the container, and  $\sigma, \sigma_i \geq 0$  are surface energies, per unit area.

Problem VP without contact energy ( $\sigma_i = 0$ ) is discussed in [Q1], where existence is established for global minimizers and, to obtain a better understanding of such minimizers, VP is solved explicitly for a square container. The theory with  $\sigma_i \neq 0$  is more interesting: for  $|\sigma_1 - \sigma_2| \leq \sigma$ , the underlying variational problem has a solution, but not generally when  $|\sigma_1 - \sigma_2| \geq \sigma$  [Q9]. This lack of existence has a definite physical meaning in terms of the limit approached by minimizing sequences. For  $\sigma_2 > \sigma_1 + \sigma$  (say), this limit

corresponds to coating the walls of the container with a "thin" layer of phase 1.

A second method of including interfacial energy is the Cahn-Hilliard theory in which the stable density distributions are characterized by the variational problem

$$P(\sigma): \text{ minimize } \int_{\Omega} \{W(u) + \sigma |\nabla u|^2\} \quad \text{subject to } \int_{\Omega} u = m.$$

Here  $W(u)$  is a nonconvex function which represents the coarse-grain free-energy of the fluid, while the term involving  $|\nabla u|^2$  is a measure of interfacial energy. With Matano (U. Hiroshima) the following results were obtained for Problem  $P(\sigma)$  [Q10]:

- (i) local minimizers belong to  $L^{\infty}(\Omega)$ ;
- (ii) for certain nice regions local minimizers exhibit relatively simple behavior; for example, in a cylinder of arbitrary cross section local minimizers are monotone in the axial direction;
- (iii) for sufficiently thin or sufficiently long regions, stationary solutions are independent of the coordinates describing the "small dimensions".

Results concerning these problems have application, not only to liquid-liquid and liquid-vapor transitions, but also to special cases of solid-solid transitions. Further,  $P(\sigma)$  characterizes stable equilibria within the dynamical theory of

Cahn [R6] (the Cahn-Hilliard theory), so that results concerning  $P(\sigma)$  have possible application to phase separation in binary alloys.

A review article [Q5] was written on phase equilibria; this article contained several conjectures which might be of interest to workers in the calculus of variations. One of the conjectures - that as  $\sigma \rightarrow 0$ , global minimizers of  $P(\sigma)$  approach the corresponding bi-constant solution of  $P(0)$  with corresponding interface a surface of minimal area at fixed phase volume - was recently proved by Modica [R7] and Sternberg [R8].

#### **Continuum mechanics**

The classical theory of fluids does not have sufficient structure to model phenomena such as capillarity, and for that reason Korteweg (cf. Truesdell and Noll [R9], Sect. 124) generalized the underlying constitutive equations by allowing the stored energy to depend not only on the density but also on the density gradient. In [Q2,Q6] the principle of virtual work is used to develop a consistent set of field equations and boundary conditions for Korteweg fluids.<sup>2</sup> This theory allows for a superficial energy on the interface between the fluid and the surrounding media; the corresponding boundary condition indicates a strong interaction between this superficial energy and the gradient dependence of the bulk

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<sup>2</sup>Cf. Dunn and Serrin [R10], who take a more general approach.

energy.

A study was completed [Q3] discussing questions of material symmetry for models of this type.

### **Viscoplasticity**

In collaboration with Browning (Los Alamos National Laboratory) and Williams (Carnegie Mellon) [R11]<sup>3</sup> we have developed a simplified constitutive theory for the one-dimensional response of certain filled polymers (such as those used in solid propellants and high explosives).<sup>4</sup> This constitutive equation isolates the rate-dependent portion of the stress response in the form of a convolution of a single stress-relaxation function with an elastic-plastic stress-strain law. A review article [Q7] concerning this model was written.

Applications to temperature-varying environments are extremely important, and consequently work was begun [Q11] on extending the theory in that direction. This study, still in its preliminary stages, is based on experiments performed at Los Alamos.

### **Nonlinear viscoelasticity**

Because of the difficulties inherent in general nonlinear

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<sup>3</sup>Partially supported under a precursor of this grant.

<sup>4</sup>This model is now being used for the solution of actual problems by the Los Alamos National Laboratory, and Lawrence Livermore Laboratory has developed (and coded) a three dimensional theory [R12] based on our model.

viscoelasticity, models have been proposed which capture the essential interaction between dissipation and nonlinearity, but are sufficiently simple to allow for the characterization of real materials and for the analysis of corresponding initial/boundary-value problems. Most such models are based on constitutive equations in single-integral form:

$$\sigma(t) = f(\epsilon(t)) + \int_0^{\infty} F(s, \epsilon(t), \epsilon(t-s)) ds. \quad (I)$$

Here  $\sigma$  is the stress and  $\epsilon$  the strain, while  $f$  and  $F$  are material functions. An energy corresponding to (I) is a single-integral law between strain  $\epsilon$  and free energy  $\psi$  such that  $\psi' \leq \sigma \epsilon'$  in any constitutive process. In collaboration [Q13] with W. Hrusa (Carnegie Mellon) we establish the existence of an energy for (I). We show that this energy is unique and give simple formulas for its construction. Such energies are important as they provide a Lyapunov function for corresponding initial/boundary-value problems. The results should have application to the dynamic analysis of polymeric materials.

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Vianello earned a Ph.D. degree while employed on the project. Milic and Struthers are currently pursuing Ph.D. degrees.

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